Relative reactivity of the metal-amido versus metal-imido bond in linked cp-amido and half-sandwich complexes of vanadium

Bouwkamp, Marco W.; Batinas, Aurora A.; Witte, Peter T.; Hubregtse, Ton; Dam, Jeroen; Meetsma, Auke; Teuben, Jan H.; Hessen, Bart

Published in:
Organometallics

DOI:
10.1021/om8003306

Publication date:
2008

```
# CIF-file generated for C46H54BN2OV                              CP883
#===============================================================================
data_global
#===============================================================================

# 0. AUDIT DETAILS

_audit_creation_date                 '2004-03-03  09:11:52'
_audit_creation_method
;
 PLATON <TABLE ACC> option
 SHELXL97-2 & Manual Editing
;
_audit_update_record
;
?

2008-04-02 # Formatted by publCIF
;

#===============================================================================

# 1. SUBMISSION DETAILS

_publ_contact_author_name           # Name  of author for correspondence
;
   Drs. A. Meetsma
;
_publ_contact_author_address        # Address of author for correspondence
;
  Crystal Structure Center, Chemical Physics,
  Zernike Institute for Advanced Materials,
  University of Groningen,
  Nijenborgh 4,
  NL-9747 AG Groningen, The Netherlands.
;
_publ_contact_author_email           A.Meetsma@rug.nl
_publ_contact_author_fax             '+31 50 3634441'
_publ_contact_author_phone           '+31 50 3634368'

_publ_requested_journal              'Organometallics'
# Publication choise FI, CI or EI for Inorganic
#                    FM, CM or EM for Metal-organic
#                    FO, CO or EO for Organic
_publ_requested_category             ?
_publ_requested_coeditor_name        ?

_publ_contact_letter                # Include date of submission
;
 Date of submission :  2008-04-02  09:11:52


 Consider this CIF submission for deposition of the first
 X-ray structure of a manuscript to be submitted to : Organometallics
  (Our Compound_Identification_Code : CP883)
;

#===============================================================================

# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)
```

```
_journal_date_recd_electronic        ?

_journal_date_to_coeditor            ?
_journal_date_from_coeditor          ?
_journal_date_accepted               ?

_journal_date_printers_first         ?
_journal_date_printers_final         ?
_journal_date_proofs_out             ?
_journal_date_proofs_in              ?

_journal_coeditor_name               ?
_journal_coeditor_code               ?
_journal_coeditor_notes
; ?
;

_journal_techeditor_code             ?
_journal_techeditor_notes
; ?
;

_journal_coden_ASTM                  ?
_journal_name_full                   ?
_journal_year                        ?
_journal_volume                      ?
_journal_issue                       ?
_journal_page_first                  ?
_journal_page_last                   ?


_journal_suppl_publ_number           ?
_journal_suppl_publ_pages            ?


#==============================================================================

# 3. TITLE AND AUTHOR LIST

_publ_section_title
;
Title (type here to add)
;
_publ_section_title_footnote
.

# The loop structure below should contain the names and adresses of all
# authors, in the required order of publication. Repeat as necessary.


loop_
_publ_author_name
_publ_author_footnote
_publ_author_address

   'Meetsma, Auke'
;
 ? # author related footnote
;
;
  Crystal Structure Center, Chemical Physics,
```

```
  Zernike Institute for Advanced Materials,
  University of Groningen,
  Nijenborgh 4,
  NL-9747 AG Groningen, The Netherlands.
;

#===============================================================================

# 4. TEXT

_publ_section_synopsis
.
_publ_section_abstract
;
(type here to add abstract)
;

# Insert blank lines between paragraphs

_publ_section_comment
;
The asymmetric unit consists of two moieties: a cationic V-complex and a
tetraphenylborate anion.
;
_publ_section_exptl_prep
;

;
_publ_section_exptl_refinement
;
The structure was solved by Patterson methods and extension of the model was
accomplished by direct methods applied to difference structure factors using
the program <i>DIRDIF</i>. The positional and anisotropic displacement
parameters for the non-hydrogen atoms were refined. Some atoms showed
unrealistic displacement parameters when allowed to vary anisotropically,
suggesting dynamic disorder (dynamic means that the smeared electron density
is due to fluctuations of the atomic positions within each unit cell). This is
in line with the weak scattering power of the crystals investigated. The
hydrogen atoms were included in the final refinement riding on their carrier
atoms with their positions calculated by using sp2 or sp3 hybridization at the
C-atom as appropriate with <i>U</i>~iso~ = c <i>x</i> Uequiv of their parent
atom, where c = 1.2 for the non-methyl hydrogen atoms and c = 1.5 for the
methyl hydrogen atoms and where values Uequiv are related to the atoms to
which the hydrogen atoms are bonded. The methyl-groups were refined as rigid
groups, which were allowed to rotate free.
;

# Insert blank lines between references

_publ_section_references
;
Beurskens, P.T., Beurskens, G., Gelder, R. de Garc\'ia-Granda, S. Gould, R.O.
Isra\"el, & Smits, J.M.M.  (1999). The <i>DIRDIF99</i> program system,
Technical Report of the Crystallography Laboratory, University of Nijmegen,
The Netherlands.

Bruker,  (2000). <i>SMART</i>, <i>SAINT</i>, <i>SADABS</i>, <i>XPREP</i> and
<i>SHELXTL</i>/NT. Software Reference Manual Bruker AXS Inc. Madison,
Wisconsin, USA.

International Tables for Crystallography  (1983). <i>Vol. A. Space-group
```

symmetry, edited by T. Hahn. Dordrecht: Reidel. (Present distributor Kluwer Academic Publishers, Dordrecht).

Meetsma, A. (2003). Extended version of the program PLUTO. Groningen University, The Netherlands. (unpublished).

Sheldrick, G. M. (1997). SHELXL97. Program for Crystal Structure Refinement. University of G\"ottingen, Germany.

Sheldrick, G. M. (2001). SADABS. Version 2.03. Multi-Scan Absorption Correction Program. University of G\"ottingen, Germany.

Spek, A. L. (1990). Acta Cryst. A46 C-34.

Spek, A. L. (1994). Am. Crystallogr. Assoc.-Abstracts, 22, 66--?.
;

_publ_section_figure_captions
;

Fig. 1. Perspective PLUTO drawing of the molecule illustrating the configuration and the adopted numbering scheme.

Fig. 2. Molecular packing viewed down unit cell axes.

Fig. 3. Perspective ORTEP drawing of the title compound. Displacement ellipsoids for non-H are represented at the 50% probability level. The H-atoms have been omitted to improve clarity.
;

#==

5. CHEMICAL DATA

_chemical_name_systematic
; ?
;
_chemical_name_common   ?
_chemical_melting_point   ?
_chemical_formula_moiety
'C22 H34 N2 O V, C24 H20 B'
Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
_chemical_formula_structural   ?
_chemical_formula_sum
'C46 H54 B N2 O V'
_chemical_formula_iupac   ?
_chemical_formula_weight   712.70
_chemical_compound_source   'see text'

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
 V   V   0.3005   0.5294
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 O   O   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

```
 N   N    0.0061    0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 B   B    0.0013    0.0007
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 H   H    0.0000    0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 C   C    0.0033    0.0016
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

#==============================================================================

# 6. CRYSTAL DATA

_symmetry_cell_setting                Triclinic
_symmetry_space_group_name_Hall      '-P 1'
_symmetry_space_group_name_H-M       'P -1'
_symmetry_Int_Tables_number                2

loop_
_symmetry_equiv_pos_as_xyz
 x,y,z
 -x,-y,-z

_cell_length_a                         9.2873(9)
_cell_length_b                        12.827(1)
_cell_length_c                        16.830(2)
_cell_angle_alpha                     93.630(2)
_cell_angle_beta                      94.974(2)
_cell_angle_gamma                    104.100(1)
_cell_volume                        1929.8(3)
_cell_formula_units_Z                  2

_cell_measurement_temperature    100(1)
_cell_measurement_reflns_used      3813
_cell_measurement_theta_min        2.44
_cell_measurement_theta_max       24.07
_cell_special_details
;
 The final unit cell was obtained from the xyz centroids of
   3813 reflections after integration using the SAINT software
   package (Bruker, 2000).
;

_exptl_crystal_description       'block'
_exptl_crystal_colour            'red'
_exptl_crystal_size_max           0.26
_exptl_crystal_size_mid           0.21
_exptl_crystal_size_min           0.16
_exptl_crystal_size_rad           ?
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.226
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              760
_exptl_absorpt_coefficient_mu     0.294
_exptl_absorpt_correction_type    'Multi-Scan'
_exptl_absorpt_process_details    '(SADABS, Sheldrick, 2001))'
_exptl_absorpt_correction_T_min   0.8591
_exptl_absorpt_correction_T_max   0.9544


#==============================================================================
```

```
# 7. EXPERIMENTAL DATA

_exptl_special_details
; ?
;
_diffrn_ambient_temperature            100(1)
_diffrn_radiation_wavelength           0.71073
_diffrn_radiation_type                'MoK\a'
_diffrn_radiation_source              'fine focus sealed Siemens Mo tube '
_diffrn_radiation_monochromator       'parallel mounted graphite'
_diffrn_radiation_detector
;
  CCD area-detector
;
_diffrn_measurement_device_type
;
  Bruker Smart Apex
;
_diffrn_measurement_method            'phi and omega scans'
_diffrn_special_details
;
 Crystal into the cold nitrogen stream of the low-temparature unit
   (KRYOFLEX, (Bruker, 2000)).
;
_diffrn_detector_area_resol_mean      66.06

_diffrn_standards_number              ?
_diffrn_standards_interval_count      ?
_diffrn_standards_interval_time       ?

loop_
_diffrn_standard_refln_index_h
_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
 ? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number              13857
_diffrn_reflns_av_R_equivalents    0.0468
_diffrn_reflns_av_sigmaI/netI      0.1040
_diffrn_reflns_limit_h_min         -11
_diffrn_reflns_limit_h_max         11
_diffrn_reflns_limit_k_min         -15
_diffrn_reflns_limit_k_max         15
_diffrn_reflns_limit_l_min         -20
_diffrn_reflns_limit_l_max         19
_diffrn_reflns_theta_min           2.44
_diffrn_reflns_theta_max           25.03
_diffrn_measured_fraction_theta_max    0.983
_diffrn_reflns_theta_full              25.00
_diffrn_measured_fraction_theta_full   0.983

_diffrn_reflns_reduction_process
;
 Intensity data were corrected for Lorentz and polarization
  effects, decay and absorption and reduced to F~o~^2^
  using SAINT (Bruker, 2000) and SADABS (Sheldrick, 2001)
;

# number of unique reflections
```

```
_reflns_number_total              6687
_reflns_number_gt                 4562
_reflns_threshold_expression      I>2\s(I)

_computing_data_collection          'SMART (Bruker, 2000)'
_computing_cell_refinement          'SAINT-Plus (Bruker, 2000)'
_computing_data_reduction           'SAINT-Plus (Bruker, 2000)'
_computing_structure_solution
;
 DIRDIF-99 (Beurskens et al., 1999)
;
_computing_structure_refinement      'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
 PLUTO (Meetsma, 2003)
 PLATON (Spek, 1994)
;
_computing_publication_material      'PLATON (Spek, 1990)'

#===============================================================================

# 8. REFINEMENT DATA

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0924P)^2^+5.22P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      heavy
_atom_sites_solution_secondary    direct
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     constr
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_abs_structure_details  ?
_chemical_absolute_configuration  ?
_refine_ls_abs_structure_Flack    ?
_refine_ls_number_reflns          6687
_refine_ls_number_parameters      465
_refine_ls_number_restraints      0
_refine_ls_number_constraints     ?
_refine_ls_R_factor_all           0.1211
_refine_ls_R_factor_gt            0.0823
_refine_ls_wR_factor_ref          0.2313
_refine_ls_wR_factor_gt           0.2059
_refine_ls_goodness_of_fit_ref    1.022
_refine_ls_restrained_S_all       1.022
_refine_ls_shift/su_max           0.000
_refine_ls_shift/su_mean          0.000
_refine_diff_density_max          0.68
```

```
_refine_diff_density_min         -0.54
_refine_diff_density_rms          0.09

_vrn_publ_code_void_volume         18.9
_vrn_publ_code_frame_time_sec      10.0
_vrn_publ_code_meas_time_hour       8.0

#===============================================================================

# 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_thermal_displace_type
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
V1 V Uani 1.02878(9) 0.34999(6) 0.29933(5) 1.000 0.0275(3) . .
O1 O Uani 0.9347(4) 0.2614(3) 0.1960(2) 1.000 0.0370(11) . .
N11 N Uani 0.9402(4) 0.2652(3) 0.3605(2) 1.000 0.0272(12) . .
N12 N Uani 0.9188(4) 0.4539(3) 0.2978(3) 1.000 0.0355(14) . .
C11 C Uani 1.2469(6) 0.3760(9) 0.3747(4) 1.000 0.073(3) . .
C12 C Uani 1.2544(6) 0.4710(5) 0.3356(5) 1.000 0.062(3) . .
C13 C Uani 1.2554(6) 0.4461(6) 0.2576(4) 1.000 0.054(2) . .
C14 C Uani 1.2489(7) 0.3406(7) 0.2448(5) 1.000 0.065(3) . .
C15 C Uani 1.2460(6) 0.2976(5) 0.3157(7) 1.000 0.070(3) . .
C16 C Uani 0.9022(5) 0.1898(4) 0.4154(3) 1.000 0.0257(14) . .
C17 C Uani 0.7871(5) 0.0976(4) 0.3942(3) 1.000 0.0339(17) . .
C18 C Uani 0.7487(6) 0.0225(4) 0.4491(3) 1.000 0.0350(17) . .
C19 C Uani 0.8237(6) 0.0358(4) 0.5247(3) 1.000 0.0293(16) . .
C110 C Uani 0.9393(5) 0.1271(4) 0.5444(3) 1.000 0.0306(17) . .
C111 C Uani 0.9787(5) 0.2035(4) 0.4916(3) 1.000 0.0304(17) . .
C112 C Uani 0.7816(7) -0.0451(4) 0.5845(3) 1.000 0.0402(19) . .
C113 C Uani 0.7824(5) 0.4512(4) 0.3405(3) 1.000 0.0372(17) . .
C114 C Uani 0.6561(6) 0.3535(5) 0.3107(5) 1.000 0.061(3) . .
C115 C Uani 0.8183(7) 0.4574(5) 0.4302(3) 1.000 0.049(2) . .
C116 C Uani 0.9626(6) 0.5528(4) 0.2561(3) 1.000 0.0407(17) . .
C117 C Uani 1.0058(6) 0.6529(4) 0.3125(4) 1.000 0.0460(19) . .
C118 C Uani 0.8418(8) 0.5603(6) 0.1911(4) 1.000 0.061(3) . .
C119 C Uani 0.9282(11) 0.2956(5) 0.1155(3) 1.000 0.084(3) . .
C120 C Uani 0.8236(8) 0.2107(5) 0.0660(3) 1.000 0.058(2) . .
C121 C Uani 0.8261(10) 0.1133(5) 0.1050(4) 1.000 0.072(3) . .
C122 C Uani 0.8651(11) 0.1475(5) 0.1891(4) 1.000 0.081(3) . .


H11 H Uiso 1.24323 0.36822 0.43028 1.000 0.0874 . .
H12 H Uiso 1.25809 0.54032 0.36050 1.000 0.0743 . .
H13 H Uiso 1.26003 0.49521 0.21740 1.000 0.0646 . .
H14 H Uiso 1.24671 0.30263 0.19414 1.000 0.0777 . .
H15 H Uiso 1.24372 0.22456 0.32347 1.000 0.0843 . .
H17 H Uiso 0.73490 0.08625 0.34207 1.000 0.0404 . .
H18 H Uiso 0.66882 -0.03963 0.43430 1.000 0.0416 . .
H110 H Uiso 0.99307 0.13706 0.59608 1.000 0.0364 . .
H111 H Uiso 1.05810 0.26577 0.50706 1.000 0.0362 . .
H112 H Uiso 0.87123 -0.06429 0.60752 1.000 0.0602 . .
H112' H Uiso 0.71066 -0.10984 0.55787 1.000 0.0602 . .
```

```
H112" H Uiso 0.73538 -0.01392 0.62716 1.000 0.0602 . .
H113 H Uiso 0.74742 0.51677 0.32810 1.000 0.0447 . .
H114 H Uiso 0.64084 0.34836 0.25204 1.000 0.0912 . .
H114' H Uiso 0.56435 0.36079 0.33256 1.000 0.0912 . .
H114" H Uiso 0.68161 0.28811 0.32806 1.000 0.0912 . .
H115 H Uiso 0.84372 0.39092 0.44497 1.000 0.0729 . .
H115' H Uiso 0.73127 0.46613 0.45644 1.000 0.0729 . .
H115" H Uiso 0.90314 0.51925 0.44735 1.000 0.0729 . .
H116 H Uiso 1.05276 0.54828 0.22897 1.000 0.0490 . .
H117 H Uiso 0.91690 0.66526 0.33497 1.000 0.0692 . .
H117' H Uiso 1.05040 0.71465 0.28353 1.000 0.0692 . .
H117" H Uiso 1.07836 0.64432 0.35585 1.000 0.0692 . .
H118 H Uiso 0.82061 0.49649 0.15260 1.000 0.0905 . .
H118' H Uiso 0.87620 0.62534 0.16340 1.000 0.0905 . .
H118" H Uiso 0.75079 0.56387 0.21540 1.000 0.0905 . .
H119 H Uiso 0.89507 0.36329 0.11489 1.000 0.1003 . .
H119' H Uiso 1.02786 0.30834 0.09585 1.000 0.1003 . .
H120 H Uiso 0.85406 0.20529 0.01125 1.000 0.0691 . .
H120' H Uiso 0.72241 0.22348 0.06261 1.000 0.0691 . .
H121 H Uiso 0.72705 0.06120 0.09592 1.000 0.0867 . .
H121' H Uiso 0.90115 0.07873 0.08402 1.000 0.0867 . .
H122 H Uiso 0.77442 0.13307 0.21772 1.000 0.0966 . .
H122' H Uiso 0.93474 0.10777 0.21284 1.000 0.0966 . .


C21 C Uani 0.4653(5) 0.9101(4) 0.1832(3) 1.000 0.0229(14) . .
C22 C Uani 0.4679(5) 0.9918(4) 0.2422(3) 1.000 0.0290(14) . .
C23 C Uani 0.4336(6) 1.0882(4) 0.2252(3) 1.000 0.0381(19) . .
C24 C Uani 0.3952(6) 1.1055(4) 0.1472(3) 1.000 0.0401(19) . .
C25 C Uani 0.3910(6) 1.0265(4) 0.0870(3) 1.000 0.0367(17) . .
C26 C Uani 0.4255(5) 0.9317(4) 0.1052(3) 1.000 0.0313(17) . .
C27 C Uani 0.4097(5) 0.6953(4) 0.1446(3) 1.000 0.0255(14) . .
C28 C Uani 0.2574(5) 0.6843(4) 0.1267(3) 1.000 0.0347(17) . .
C29 C Uani 0.1657(6) 0.5939(6) 0.0794(3) 1.000 0.0515(19) . .
C210 C Uani 0.2232(8) 0.5135(5) 0.0513(3) 1.000 0.057(2) . .
C211 C Uani 0.3699(7) 0.5187(5) 0.0691(3) 1.000 0.0483(19) . .
C212 C Uani 0.4602(6) 0.6079(4) 0.1152(3) 1.000 0.0334(17) . .
C213 C Uani 0.6898(5) 0.8252(3) 0.1744(3) 1.000 0.0209(12) . .
C214 C Uani 0.7199(5) 0.8076(4) 0.0950(3) 1.000 0.0294(16) . .
C215 C Uani 0.8613(6) 0.8351(4) 0.0712(3) 1.000 0.0375(17) . .
C216 C Uani 0.9828(5) 0.8810(4) 0.1265(3) 1.000 0.0372(19) . .
C217 C Uani 0.9590(5) 0.9007(4) 0.2048(3) 1.000 0.0354(18) . .
C218 C Uani 0.8157(5) 0.8736(3) 0.2280(3) 1.000 0.0247(12) . .
C219 C Uani 0.5107(5) 0.7688(3) 0.2926(3) 1.000 0.0210(12) . .
C220 C Uani 0.6080(5) 0.7151(4) 0.3297(3) 1.000 0.0251(12) . .
C221 C Uani 0.6004(5) 0.6852(4) 0.4068(3) 1.000 0.0302(17) . .
C222 C Uani 0.4961(5) 0.7102(4) 0.4521(3) 1.000 0.0262(12) . .
C223 C Uani 0.3948(5) 0.7600(4) 0.4182(3) 1.000 0.0274(14) . .
C224 C Uani 0.4016(5) 0.7876(3) 0.3404(3) 1.000 0.0244(14) . .
B2 B Uani 0.5186(5) 0.7992(4) 0.1999(3) 1.000 0.0209(17) . .


H22 H Uiso 0.49432 0.98130 0.29638 1.000 0.0344 . .
H23 H Uiso 0.43669 1.14188 0.26733 1.000 0.0454 . .
H24 H Uiso 0.37187 1.17123 0.13497 1.000 0.0483 . .
H25 H Uiso 0.36433 1.03742 0.03296 1.000 0.0437 . .
H26 H Uiso 0.42216 0.87843 0.06272 1.000 0.0369 . .
H28 H Uiso 0.21400 0.73913 0.14686 1.000 0.0416 . .
H29 H Uiso 0.06248 0.58949 0.06719 1.000 0.0623 . .
H210 H Uiso 0.16065 0.45332 0.01907 1.000 0.0683 . .
H211 H Uiso 0.41051 0.46173 0.05019 1.000 0.0582 . .
```

```
H212 H Uiso 0.56258 0.60966 0.12758 1.000 0.0398 . .
H214 H Uiso 0.63869 0.77517 0.05584 1.000 0.0350 . .
H215 H Uiso 0.87553 0.82260 0.01650 1.000 0.0450 . .
H216 H Uiso 1.08095 0.89849 0.11063 1.000 0.0449 . .
H217 H Uiso 1.04121 0.93308 0.24339 1.000 0.0426 . .
H218 H Uiso 0.80255 0.88865 0.28247 1.000 0.0290 . .
H220 H Uiso 0.68345 0.69819 0.30035 1.000 0.0301 . .
H221 H Uiso 0.66805 0.64705 0.42863 1.000 0.0362 . .
H222 H Uiso 0.49412 0.69322 0.50618 1.000 0.0312 . .
H223 H Uiso 0.31948 0.77568 0.44817 1.000 0.0327 . .
H224 H Uiso 0.32865 0.82109 0.31816 1.000 0.0292 . .


loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
V1 0.0282(5) 0.0272(5) 0.0273(5) 0.0023(3) 0.0021(3) 0.0075(3)
O1 0.045(2) 0.0242(17) 0.038(2) 0.0094(15) 0.0014(16) 0.0006(15)
N11 0.025(2) 0.028(2) 0.029(2) 0.0014(17) 0.0023(17) 0.0079(17)
N12 0.030(2) 0.039(2) 0.040(3) 0.002(2) 0.0038(19) 0.0139(19)
C11 0.022(3) 0.162(9) 0.033(4) 0.035(5) 0.000(2) 0.014(4)
C12 0.026(3) 0.046(4) 0.104(6) -0.036(4) -0.012(3) 0.008(3)
C13 0.033(3) 0.073(5) 0.061(4) 0.038(4) 0.014(3) 0.012(3)
C14 0.034(3) 0.093(6) 0.068(5) -0.020(4) 0.011(3) 0.021(4)
C15 0.026(3) 0.039(4) 0.154(9) 0.040(5) 0.012(4) 0.014(3)
C16 0.027(2) 0.025(2) 0.028(3) 0.007(2) 0.009(2) 0.009(2)
C17 0.036(3) 0.039(3) 0.024(3) 0.006(2) 0.001(2) 0.004(2)
C18 0.037(3) 0.029(3) 0.036(3) 0.004(2) 0.004(2) 0.002(2)
C19 0.043(3) 0.027(2) 0.025(3) 0.005(2) 0.012(2) 0.019(2)
C110 0.036(3) 0.032(3) 0.024(3) 0.002(2) 0.001(2) 0.010(2)
C111 0.031(3) 0.031(3) 0.028(3) 0.003(2) 0.005(2) 0.005(2)
C112 0.061(4) 0.032(3) 0.033(3) 0.009(2) 0.012(3) 0.018(3)
C113 0.027(3) 0.038(3) 0.051(3) 0.004(2) 0.012(2) 0.014(2)
C114 0.034(3) 0.046(4) 0.101(6) 0.006(4) 0.001(3) 0.010(3)
C115 0.058(4) 0.044(3) 0.051(4) 0.008(3) 0.019(3) 0.021(3)
C116 0.040(3) 0.052(3) 0.042(3) 0.023(3) 0.017(3) 0.025(3)
C117 0.035(3) 0.039(3) 0.066(4) 0.014(3) 0.002(3) 0.012(2)
C118 0.079(5) 0.083(5) 0.037(3) 0.012(3) 0.007(3) 0.052(4)
C119 0.171(8) 0.041(4) 0.019(3) 0.007(3) -0.007(4) -0.007(4)
C120 0.080(5) 0.066(4) 0.024(3) 0.001(3) 0.001(3) 0.015(4)
C121 0.108(6) 0.046(4) 0.041(4) -0.002(3) -0.003(4) -0.016(4)
C122 0.164(8) 0.025(3) 0.031(3) -0.001(3) -0.011(4) -0.012(4)
C21 0.016(2) 0.028(2) 0.028(3) 0.008(2) 0.0074(18) 0.0087(18)
C22 0.027(2) 0.028(2) 0.034(3) 0.005(2) 0.006(2) 0.009(2)
C23 0.040(3) 0.026(3) 0.053(4) 0.006(2) 0.015(3) 0.013(2)
C24 0.042(3) 0.033(3) 0.057(4) 0.019(3) 0.019(3) 0.023(2)
C25 0.041(3) 0.039(3) 0.037(3) 0.019(2) 0.011(2) 0.017(2)
C26 0.033(3) 0.034(3) 0.031(3) 0.009(2) 0.009(2) 0.013(2)
C27 0.020(2) 0.032(3) 0.021(2) 0.008(2) -0.0021(18) 0.000(2)
C28 0.028(3) 0.042(3) 0.031(3) 0.018(2) -0.005(2) 0.002(2)
C29 0.027(3) 0.074(4) 0.039(3) 0.033(3) -0.015(2) -0.016(3)
C210 0.064(4) 0.052(4) 0.034(3) 0.003(3) -0.008(3) -0.022(3)
C211 0.062(4) 0.037(3) 0.034(3) -0.009(2) 0.007(3) -0.008(3)
C212 0.035(3) 0.029(3) 0.031(3) 0.000(2) 0.003(2) -0.001(2)
C213 0.020(2) 0.019(2) 0.025(2) 0.0018(18) 0.0008(18) 0.0081(18)
C214 0.024(2) 0.033(3) 0.032(3) 0.005(2) 0.004(2) 0.008(2)
```

```
C215 0.036(3) 0.045(3) 0.037(3) 0.010(2) 0.019(2) 0.014(2)
C216 0.022(3) 0.036(3) 0.057(4) 0.014(3) 0.016(2) 0.007(2)
C217 0.020(2) 0.033(3) 0.053(4) 0.006(2) -0.002(2) 0.008(2)
C218 0.024(2) 0.026(2) 0.024(2) 0.0001(19) -0.0009(19) 0.0080(19)
C219 0.017(2) 0.021(2) 0.023(2) -0.0006(18) 0.0003(18) 0.0025(17)
C220 0.026(2) 0.030(2) 0.024(2) 0.003(2) 0.0046(19) 0.015(2)
C221 0.029(3) 0.032(3) 0.032(3) 0.008(2) -0.002(2) 0.013(2)
C222 0.029(2) 0.029(2) 0.018(2) 0.0024(19) -0.0004(19) 0.003(2)
C223 0.027(2) 0.027(2) 0.028(3) -0.001(2) 0.007(2) 0.006(2)
C224 0.018(2) 0.023(2) 0.033(3) 0.003(2) -0.0023(19) 0.0085(18)
B2 0.023(3) 0.024(3) 0.019(3) 0.002(2) 0.003(2) 0.012(2)

#===============================================================================

# 10. MOLECULAR GEOMETRY

_geom_special_details
;
 Bond distances, angles etc. have been calculated using the
 rounded fractional coordinates. All su's are estimated
 from the variances of the (full) variance-covariance matrix.
 The cell esds are taken into account in the estimation of
 distances, angles and torsion angles
;

loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
 V1      O1         2.020(4)                    .      .                   yes
 V1      N11        1.665(4)                    .      .                   yes
 V1      N12        1.866(4)                    .      .                   yes
 V1      C11        2.235(7)                    .      .                   yes
 V1      C12        2.290(6)                    .      .                   yes
 V1      C13        2.355(7)                    .      .                   yes
 V1      C14        2.338(7)                    .      .                   yes
 V1      C15        2.277(6)                    .      .                   yes
 O1      C119       1.451(6)                    .      .                   yes
 O1      C122       1.439(7)                    .      .                   yes
 N11     C16        1.385(6)                    .      .                   yes
 N12     C113       1.504(6)                    .      .                   yes
 N12     C116       1.476(6)                    .      .                   yes
 C11     C12       1.411(12)                    .      .                   no
 C11     C15       1.366(13)                    .      .                   no
 C12     C13       1.333(11)                    .      .                   no
 C13     C14       1.343(11)                    .      .                   no
 C14     C15       1.346(14)                    .      .                   no
 C16     C17        1.390(7)                    .      .                   no
 C16     C111       1.390(7)                    .      .                   no
 C17     C18        1.383(7)                    .      .                   no
 C18     C19        1.376(7)                    .      .                   no
 C19     C110       1.382(7)                    .      .                   no
 C19     C112       1.499(7)                    .      .                   no
 C110    C111       1.370(7)                    .      .                   no
 C11     H11          0.9496                    .      .                   no
 C12     H12          0.9502                    .      .                   no
 C13     H13          0.9499                    .      .                   no
 C113    C114       1.517(8)                    .      .                   no
```

C113	C115	1.510(7)	.	.	no
C14	H14	0.9509	.	.	no
C15	H15	0.9495	.	.	no
C116	C117	1.496(8)	.	.	no
C116	C118	1.522(9)	.	.	no
C17	H17	0.9495	.	.	no
C18	H18	0.9499	.	.	no
C119	C120	1.433(9)	.	.	no
C120	C121	1.452(9)	.	.	no
C121	C122	1.443(9)	.	.	no
C110	H110	0.9496	.	.	no
C111	H111	0.9502	.	.	no
C112	H112'	0.9796	.	.	no
C112	H112"	0.9800	.	.	no
C112	H112	0.9796	.	.	no
C113	H113	1.0000	.	.	no
C114	H114'	0.9793	.	.	no
C114	H114"	0.9802	.	.	no
C114	H114	0.9808	.	.	no
C115	H115'	0.9801	.	.	no
C115	H115"	0.9801	.	.	no
C115	H115	0.9795	.	.	no
C116	H116	0.9998	.	.	no
C117	H117'	0.9802	.	.	no
C117	H117"	0.9796	.	.	no
C117	H117	0.9799	.	.	no
C118	H118'	0.9801	.	.	no
C118	H118"	0.9799	.	.	no
C118	H118	0.9802	.	.	no
C119	H119'	0.9894	.	.	no
C119	H119	0.9896	.	.	no
C120	H120'	0.9901	.	.	no
C120	H120	0.9902	.	.	no
C121	H121'	0.9902	.	.	no
C121	H121	0.9896	.	.	no
C21	C26	1.396(7)	.	.	no
C21	B2	1.648(7)	.	.	yes
C21	C22	1.392(7)	.	.	no
C122	H122'	0.9896	.	.	no
C122	H122	0.9906	.	.	no
C22	C23	1.390(7)	.	.	no
C23	C24	1.376(7)	.	.	no
C24	C25	1.378(7)	.	.	no
C25	C26	1.377(7)	.	.	no
C27	C28	1.391(7)	.	.	no
C27	B2	1.640(7)	.	.	yes
C27	C212	1.396(7)	.	.	no
C28	C29	1.410(8)	.	.	no
C29	C210	1.350(9)	.	.	no
C22	H22	0.9501	.	.	no
C23	H23	0.9501	.	.	no
C24	H24	0.9505	.	.	no
C25	H25	0.9498	.	.	no
C26	H26	0.9502	.	.	no
C28	H28	0.9507	.	.	no
C29	H29	0.9499	.	.	no
C210	C211	1.354(10)	.	.	no
C211	C212	1.386(8)	.	.	no
C213	C218	1.400(7)	.	.	no
C213	C214	1.404(7)	.	.	no
C213	B2	1.644(7)	.	.	yes

```
 C214    C215       1.376(7)                    .      .                 no
 C215    C216       1.382(7)                    .      .                 no
 C216    C217       1.373(7)                    .      .                 no
 C217    C218       1.388(7)                    .      .                 no
 C219    C220       1.393(7)                    .      .                 no
 C219    C224       1.403(7)                    .      .                 no
 C219    B2         1.635(7)                    .      .                 yes
 C220    C221       1.379(7)                    .      .                 no
 C221    C222       1.368(7)                    .      .                 no
 C222    C223       1.366(7)                    .      .                 no
 C223    C224       1.381(7)                    .      .                 no
 C210    H210         0.9494                    .      .                 no
 C211    H211         0.9504                    .      .                 no
 C212    H212         0.9501                    .      .                 no
 C214    H214         0.9500                    .      .                 no
 C215    H215         0.9505                    .      .                 no
 C216    H216         0.9501                    .      .                 no
 C217    H217         0.9501                    .      .                 no
 C218    H218         0.9492                    .      .                 no
 C220    H220         0.9500                    .      .                 no
 C221    H221         0.9496                    .      .                 no
 C222    H222         0.9499                    .      .                 no
 C223    H223         0.9493                    .      .                 no
 C224    H224         0.9497                    .      .                 no

loop_
_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
 O1      V1      N11       96.60(16)              .      .      .          yes
 O1      V1      N12       98.96(18)              .      .      .          yes
 O1      V1      C11        135.0(2)              .      .      .          yes
 O1      V1      C12        133.2(2)              .      .      .          yes
 O1      V1      C13        100.0(2)              .      .      .          yes
 O1      V1      C14         82.1(2)              .      .      .          yes
 O1      V1      C15         99.9(3)              .      .      .          yes
 N11     V1      N12      101.86(19)              .      .      .          yes
 N11     V1      C11         92.2(3)              .      .      .          yes
 N11     V1      C12        123.8(2)              .      .      .          yes
 N11     V1      C13        148.9(2)              .      .      .          yes
 N11     V1      C14        125.9(3)              .      .      .          yes
 N11     V1      C15         95.2(3)              .      .      .          yes
 N12     V1      C11        122.2(3)              .      .      .          yes
 N12     V1      C12         95.0(2)              .      .      .          yes
 N12     V1      C13        101.3(2)              .      .      .          yes
 N12     V1      C14        132.0(3)              .      .      .          yes
 N12     V1      C15        152.8(2)              .      .      .          yes
 C11     V1      C12         36.3(3)              .      .      .          yes
 C11     V1      C13         57.7(3)              .      .      .          yes
 C11     V1      C14         57.7(3)              .      .      .          yes
 C11     V1      C15         35.2(3)              .      .      .          yes
 C12     V1      C13         33.3(3)              .      .      .          yes
 C12     V1      C14         56.2(3)              .      .      .          yes
 C12     V1      C15         57.9(2)              .      .      .          yes
 C13     V1      C14         33.2(3)              .      .      .          yes
 C13     V1      C15         56.2(3)              .      .      .          yes
```

C14	V1	C15	33.9(3)	.	.	.	yes
V1	O1	C119	128.5(3)	.	.	.	yes
V1	O1	C122	124.9(3)	.	.	.	yes
C119	O1	C122	106.6(4)	.	.	.	yes
V1	N11	C16	165.3(4)	.	.	.	yes
V1	N12	C113	125.6(3)	.	.	.	yes
V1	N12	C116	122.4(3)	.	.	.	yes
C113	N12	C116	112.0(4)	.	.	.	yes
V1	C11	C12	74.0(4)	.	.	.	yes
V1	C11	C15	74.1(4)	.	.	.	yes
C12	C11	C15	105.4(7)	.	.	.	no
V1	C12	C11	69.7(4)	.	.	.	yes
V1	C12	C13	76.0(4)	.	.	.	yes
C11	C12	C13	107.8(6)	.	.	.	no
V1	C13	C12	70.7(4)	.	.	.	yes
V1	C13	C14	72.7(4)	.	.	.	yes
C12	C13	C14	109.2(7)	.	.	.	no
V1	C14	C13	74.1(4)	.	.	.	yes
V1	C14	C15	70.6(4)	.	.	.	yes
C13	C14	C15	108.5(7)	.	.	.	no
V1	C15	C11	70.7(4)	.	.	.	yes
V1	C15	C14	75.6(4)	.	.	.	yes
C11	C15	C14	109.0(7)	.	.	.	no
N11	C16	C17	119.9(4)	.	.	.	yes
N11	C16	C111	121.2(4)	.	.	.	yes
C17	C16	C111	118.9(5)	.	.	.	no
C16	C17	C18	119.9(5)	.	.	.	no
C17	C18	C19	121.4(5)	.	.	.	no
C18	C19	C110	117.9(5)	.	.	.	no
C18	C19	C112	121.5(5)	.	.	.	no
C110	C19	C112	120.6(5)	.	.	.	no
C19	C110	C111	122.0(5)	.	.	.	no
C16	C111	C110	119.9(5)	.	.	.	no
V1	C11	H11	117.01	.	.	.	no
C12	C11	H11	127.28	.	.	.	no
C15	C11	H11	127.29	.	.	.	no
C13	C12	H12	126.16	.	.	.	no
C11	C12	H12	126.05	.	.	.	no
V1	C12	H12	119.98	.	.	.	no
C114	C113	C115	111.3(5)	.	.	.	no
N12	C113	C115	111.5(4)	.	.	.	yes
N12	C113	C114	111.8(4)	.	.	.	yes
V1	C13	H13	122.85	.	.	.	no
C14	C13	H13	125.36	.	.	.	no
C12	C13	H13	125.41	.	.	.	no
C13	C14	H14	125.74	.	.	.	no
C15	C14	H14	125.72	.	.	.	no
V1	C14	H14	121.33	.	.	.	no
C11	C15	H15	125.50	.	.	.	no
C14	C15	H15	125.52	.	.	.	no
V1	C15	H15	119.95	.	.	.	no
N12	C116	C117	112.5(4)	.	.	.	yes
N12	C116	C118	111.8(5)	.	.	.	yes
C117	C116	C118	110.8(5)	.	.	.	no
C16	C17	H17	120.02	.	.	.	no
C18	C17	H17	120.04	.	.	.	no
C19	C18	H18	119.30	.	.	.	no
C17	C18	H18	119.26	.	.	.	no
O1	C119	C120	107.0(5)	.	.	.	yes
C119	C120	C121	105.0(5)	.	.	.	no
C120	C121	C122	105.7(5)	.	.	.	no

O1	C122	C121	107.5(5)	.	.	.	yes
C19	C110	H110	118.97	.	.	.	no
C111	C110	H110	119.05	.	.	.	no
C16	C111	H111	120.09	.	.	.	no
C110	C111	H111	120.04	.	.	.	no
C19	C112	H112'	109.43	.	.	.	no
C19	C112	H112"	109.43	.	.	.	no
C19	C112	H112	109.44	.	.	.	no
H112'	C112	H112"	109.49	.	.	.	no
H112'	C112	H112	109.54	.	.	.	no
H112"	C112	H112	109.50	.	.	.	no
N12	C113	H113	107.32	.	.	.	no
C114	C113	H113	107.35	.	.	.	no
C115	C113	H113	107.31	.	.	.	no
C113	C114	H114'	109.55	.	.	.	no
C113	C114	H114"	109.49	.	.	.	no
C113	C114	H114	109.43	.	.	.	no
H114'	C114	H114"	109.50	.	.	.	no
H114'	C114	H114	109.47	.	.	.	no
H114"	C114	H114	109.39	.	.	.	no
C113	C115	H115'	109.44	.	.	.	no
C113	C115	H115"	109.46	.	.	.	no
C113	C115	H115	109.47	.	.	.	no
H115'	C115	H115"	109.46	.	.	.	no
H115'	C115	H115	109.50	.	.	.	no
H115"	C115	H115	109.50	.	.	.	no
N12	C116	H116	107.17	.	.	.	no
C117	C116	H116	107.13	.	.	.	no
C118	C116	H116	107.09	.	.	.	no
C116	C117	H117'	109.45	.	.	.	no
C116	C117	H117"	109.45	.	.	.	no
C116	C117	H117	109.46	.	.	.	no
H117'	C117	H117"	109.49	.	.	.	no
H117'	C117	H117	109.46	.	.	.	no
H117"	C117	H117	109.52	.	.	.	no
C116	C118	H118'	109.49	.	.	.	no
C116	C118	H118"	109.50	.	.	.	no
C116	C118	H118	109.47	.	.	.	no
H118'	C118	H118"	109.46	.	.	.	no
H118'	C118	H118	109.45	.	.	.	no
H118"	C118	H118	109.46	.	.	.	no
O1	C119	H119'	110.28	.	.	.	no
O1	C119	H119	110.27	.	.	.	no
C120	C119	H119'	110.33	.	.	.	no
C120	C119	H119	110.31	.	.	.	no
H119'	C119	H119	108.63	.	.	.	no
C119	C120	H120'	110.79	.	.	.	no
C119	C120	H120	110.75	.	.	.	no
C121	C120	H120'	110.73	.	.	.	no
C121	C120	H120	110.75	.	.	.	no
H120'	C120	H120	108.82	.	.	.	no
C120	C121	H121'	110.55	.	.	.	no
C120	C121	H121	110.60	.	.	.	no
C122	C121	H121'	110.57	.	.	.	no
C122	C121	H121	110.65	.	.	.	no
H121'	C121	H121	108.75	.	.	.	no
C26	C21	B2	120.4(4)	.	.	.	yes
C22	C21	C26	115.1(5)	.	.	.	no
C22	C21	B2	124.2(4)	.	.	.	yes
O1	C122	H122	110.18	.	.	.	no
H122'	C122	H122	108.49	.	.	.	no

C121	C122	H122'	110.27	.	.	.	no
C121	C122	H122	110.19	.	.	.	no
O1	C122	H122'	110.22	.	.	.	no
C21	C22	C23	122.8(5)	.	.	.	no
C22	C23	C24	119.8(5)	.	.	.	no
C23	C24	C25	119.3(5)	.	.	.	no
C24	C25	C26	120.0(5)	.	.	.	no
C21	C26	C25	123.1(5)	.	.	.	no
C28	C27	C212	114.4(5)	.	.	.	no
C28	C27	B2	122.7(4)	.	.	.	yes
C212	C27	B2	122.9(4)	.	.	.	yes
C27	C28	C29	121.7(5)	.	.	.	no
C28	C29	C210	120.6(6)	.	.	.	no
C21	C22	H22	118.62	.	.	.	no
C23	C22	H22	118.61	.	.	.	no
C22	C23	H23	120.05	.	.	.	no
C24	C23	H23	120.19	.	.	.	no
C23	C24	H24	120.38	.	.	.	no
C25	C24	H24	120.35	.	.	.	no
C24	C25	H25	120.04	.	.	.	no
C26	C25	H25	119.99	.	.	.	no
C21	C26	H26	118.38	.	.	.	no
C25	C26	H26	118.54	.	.	.	no
C29	C28	H28	119.14	.	.	.	no
C27	C28	H28	119.18	.	.	.	no
C28	C29	H29	119.71	.	.	.	no
C210	C29	H29	119.67	.	.	.	no
C29	C210	C211	120.0(6)	.	.	.	no
C210	C211	C212	119.3(6)	.	.	.	no
C27	C212	C211	123.9(5)	.	.	.	no
C214	C213	C218	114.6(4)	.	.	.	no
C218	C213	B2	123.2(4)	.	.	.	yes
C214	C213	B2	122.0(4)	.	.	.	yes
C213	C214	C215	123.2(5)	.	.	.	no
C214	C215	C216	120.3(5)	.	.	.	no
C215	C216	C217	118.8(5)	.	.	.	no
C216	C217	C218	120.5(5)	.	.	.	no
C213	C218	C217	122.7(5)	.	.	.	no
C220	C219	B2	122.2(4)	.	.	.	yes
C220	C219	C224	113.7(4)	.	.	.	no
C224	C219	B2	124.0(4)	.	.	.	yes
C219	C220	C221	123.4(5)	.	.	.	no
C220	C221	C222	120.4(5)	.	.	.	no
C221	C222	C223	118.8(5)	.	.	.	no
C222	C223	C224	120.2(5)	.	.	.	no
C219	C224	C223	123.4(4)	.	.	.	no
C29	C210	H210	119.93	.	.	.	no
C211	C210	H210	120.05	.	.	.	no
C212	C211	H211	120.36	.	.	.	no
C210	C211	H211	120.30	.	.	.	no
C27	C212	H212	118.00	.	.	.	no
C211	C212	H212	118.08	.	.	.	no
C213	C214	H214	118.40	.	.	.	no
C215	C214	H214	118.43	.	.	.	no
C216	C215	H215	119.84	.	.	.	no
C214	C215	H215	119.89	.	.	.	no
C215	C216	H216	120.62	.	.	.	no
C217	C216	H216	120.63	.	.	.	no
C218	C217	H217	119.76	.	.	.	no
C216	C217	H217	119.77	.	.	.	no
C213	C218	H218	118.65	.	.	.	no

```
 C217    C218    H218         118.61             .      .      .          no
 C219    C220    H220         118.29             .      .      .          no
 C221    C220    H220         118.32             .      .      .          no
 C222    C221    H221         119.75             .      .      .          no
 C220    C221    H221         119.81             .      .      .          no
 C221    C222    H222         120.61             .      .      .          no
 C223    C222    H222         120.56             .      .      .          no
 C222    C223    H223         119.95             .      .      .          no
 C224    C223    H223         119.89             .      .      .          no
 C223    C224    H224         118.24             .      .      .          no
 C219    C224    H224         118.37             .      .      .          no
 C21     B2      C213       103.6(3)             .      .      .          yes
 C21     B2      C219       113.2(4)             .      .      .          yes
 C27     B2      C219       106.0(4)             .      .      .          yes
 C213    B2      C219       112.3(4)             .      .      .          yes
 C27     B2      C213       111.3(4)             .      .      .          yes
 C21     B2      C27        110.5(4)             .      .      .          yes

loop_
_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
 N11     V1      O1      C119       162.5(6)     .      .      .      .   no
 N11     V1      O1      C122       -20.4(6)     .      .      .      .   no
 N12     V1      O1      C119        59.3(6)     .      .      .      .   no
 N12     V1      O1      C122      -123.5(6)     .      .      .      .   no
 C11     V1      O1      C119       -97.7(7)     .      .      .      .   no
 C11     V1      O1      C122        79.5(7)     .      .      .      .   no
 C12     V1      O1      C119       -46.3(7)     .      .      .      .   no
 C12     V1      O1      C122       130.9(6)     .      .      .      .   no
 C13     V1      O1      C119       -43.9(6)     .      .      .      .   no
 C13     V1      O1      C122       133.2(6)     .      .      .      .   no
 C14     V1      O1      C119       -72.1(6)     .      .      .      .   no
 C14     V1      O1      C122       105.0(6)     .      .      .      .   no
 C15     V1      O1      C119      -101.1(6)     .      .      .      .   no
 C15     V1      O1      C122        76.1(6)     .      .      .      .   no
 O1      V1      N12     C113        96.5(4)     .      .      .      .   no
 O1      V1      N12     C116       -86.5(4)     .      .      .      .   no
 N11     V1      N12     C113        -2.3(4)     .      .      .      .   no
 N11     V1      N12     C116       174.8(4)     .      .      .      .   no
 C11     V1      N12     C113      -102.6(4)     .      .      .      .   no
 C11     V1      N12     C116        74.5(5)     .      .      .      .   no
 C12     V1      N12     C113      -128.3(4)     .      .      .      .   no
 C12     V1      N12     C116        48.7(4)     .      .      .      .   no
 C13     V1      N12     C113      -161.4(4)     .      .      .      .   no
 C13     V1      N12     C116        15.7(4)     .      .      .      .   no
 C14     V1      N12     C113      -176.1(4)     .      .      .      .   no
 C14     V1      N12     C116         1.0(6)     .      .      .      .   no
 C15     V1      N12     C113      -130.0(7)     .      .      .      .   no
 C15     V1      N12     C116        47.1(9)     .      .      .      .   no
 O1      V1      C11     C12        105.9(5)     .      .      .      .   no
 O1      V1      C11     C15         -5.8(7)     .      .      .      .   no
 N11     V1      C11     C12       -152.5(4)     .      .      .      .   no
 N11     V1      C11     C15         95.9(5)     .      .      .      .   no
```

N12	V1	C11	C12	-46.9(5)	.	.	.	.	no
N12	V1	C11	C15	-158.6(5)	.	.	.	.	no
C12	V1	C11	C15	-111.7(6)	.	.	.	.	no
C13	V1	C11	C12	36.0(4)	.	.	.	.	no
C13	V1	C11	C15	-75.8(5)	.	.	.	.	no
C14	V1	C11	C12	75.5(5)	.	.	.	.	no
C14	V1	C11	C15	-36.2(5)	.	.	.	.	no
C15	V1	C11	C12	111.7(6)	.	.	.	.	no
O1	V1	C12	C11	-111.1(4)	.	.	.	.	no
O1	V1	C12	C13	4.2(5)	.	.	.	.	no
N11	V1	C12	C11	33.8(5)	.	.	.	.	no
N11	V1	C12	C13	149.1(4)	.	.	.	.	no
N12	V1	C12	C11	141.6(4)	.	.	.	.	no
N12	V1	C12	C13	-103.0(4)	.	.	.	.	no
C11	V1	C12	C13	115.3(6)	.	.	.	.	no
C13	V1	C12	C11	-115.3(6)	.	.	.	.	no
C14	V1	C12	C11	-79.8(5)	.	.	.	.	no
C14	V1	C12	C13	35.5(4)	.	.	.	.	no
C15	V1	C12	C11	-39.3(5)	.	.	.	.	no
C15	V1	C12	C13	76.1(5)	.	.	.	.	no
O1	V1	C13	C12	-176.9(4)	.	.	.	.	no
O1	V1	C13	C14	-58.6(5)	.	.	.	.	no
N11	V1	C13	C12	-55.7(6)	.	.	.	.	no
N11	V1	C13	C14	62.6(6)	.	.	.	.	no
N12	V1	C13	C12	81.8(4)	.	.	.	.	no
N12	V1	C13	C14	-159.9(5)	.	.	.	.	no
C11	V1	C13	C12	-39.3(5)	.	.	.	.	no
C11	V1	C13	C14	79.1(5)	.	.	.	.	no
C12	V1	C13	C14	118.3(6)	.	.	.	.	no
C14	V1	C13	C12	-118.3(6)	.	.	.	.	no
C15	V1	C13	C12	-81.6(5)	.	.	.	.	no
C15	V1	C13	C14	36.8(5)	.	.	.	.	no
O1	V1	C14	C13	122.0(4)	.	.	.	.	no
O1	V1	C14	C15	-121.2(5)	.	.	.	.	no
N11	V1	C14	C13	-145.5(4)	.	.	.	.	no
N11	V1	C14	C15	-28.7(6)	.	.	.	.	no
N12	V1	C14	C13	27.0(6)	.	.	.	.	no
N12	V1	C14	C15	143.8(5)	.	.	.	.	no
C11	V1	C14	C13	-79.2(5)	.	.	.	.	no
C11	V1	C14	C15	37.7(5)	.	.	.	.	no
C12	V1	C14	C13	-35.6(4)	.	.	.	.	no
C12	V1	C14	C15	81.3(5)	.	.	.	.	no
C13	V1	C14	C15	116.8(7)	.	.	.	.	no
C15	V1	C14	C13	-116.8(7)	.	.	.	.	no
O1	V1	C15	C11	175.9(5)	.	.	.	.	no
O1	V1	C15	C14	59.4(5)	.	.	.	.	no
N11	V1	C15	C11	-86.5(5)	.	.	.	.	no
N11	V1	C15	C14	157.0(5)	.	.	.	.	no
N12	V1	C15	C11	42.5(10)	.	.	.	.	no
N12	V1	C15	C14	-74.0(9)	.	.	.	.	no
C11	V1	C15	C14	-116.5(7)	.	.	.	.	no
C12	V1	C15	C11	40.5(5)	.	.	.	.	no
C12	V1	C15	C14	-76.0(5)	.	.	.	.	no
C13	V1	C15	C11	80.4(5)	.	.	.	.	no
C13	V1	C15	C14	-36.1(5)	.	.	.	.	no
C14	V1	C15	C11	116.5(7)	.	.	.	.	no
V1	O1	C119	C120	-167.9(4)	.	.	.	.	no
C119	O1	C122	C121	3.4(9)	.	.	.	.	no
C122	O1	C119	C120	14.6(9)	.	.	.	.	no
V1	O1	C122	C121	-174.2(5)	.	.	.	.	no
V1	N12	C113	C115	63.4(5)	.	.	.	.	no

C116	N12	C113	C114	120.8(5)	.	.	.	no
C116	N12	C113	C115	-113.9(5)	.	.	.	no
V1	N12	C113	C114	-61.9(6)	.	.	.	no
C113	N12	C116	C117	63.0(6)	.	.	.	no
C113	N12	C116	C118	-62.4(6)	.	.	.	no
V1	N12	C116	C117	-114.4(5)	.	.	.	no
V1	N12	C116	C118	120.2(5)	.	.	.	no
C15	C11	C12	C13	0.9(7)	.	.	.	no
V1	C11	C12	C13	-67.1(5)	.	.	.	no
C15	C11	C12	V1	67.9(5)	.	.	.	no
C12	C11	C15	C14	-1.5(7)	.	.	.	no
V1	C11	C15	C14	66.4(5)	.	.	.	no
C12	C11	C15	V1	-67.9(4)	.	.	.	no
C11	C12	C13	C14	0.0(7)	.	.	.	no
V1	C12	C13	C14	-62.9(5)	.	.	.	no
C11	C12	C13	V1	62.9(4)	.	.	.	no
C12	C13	C14	C15	-0.9(8)	.	.	.	no
V1	C13	C14	C15	-62.6(5)	.	.	.	no
C12	C13	C14	V1	61.6(5)	.	.	.	no
C13	C14	C15	V1	64.8(5)	.	.	.	no
C13	C14	C15	C11	1.5(8)	.	.	.	no
V1	C14	C15	C11	-63.3(5)	.	.	.	no
C111	C16	C17	C18	1.2(7)	.	.	.	no
C17	C16	C111	C110	-0.5(7)	.	.	.	no
N11	C16	C17	C18	-179.7(5)	.	.	.	no
N11	C16	C111	C110	-179.5(4)	.	.	.	no
C16	C17	C18	C19	-1.0(8)	.	.	.	no
C17	C18	C19	C112	179.6(5)	.	.	.	no
C17	C18	C19	C110	0.1(8)	.	.	.	no
C112	C19	C110	C111	-178.8(5)	.	.	.	no
C18	C19	C110	C111	0.7(8)	.	.	.	no
H110	C110	C111	C16	179.38	.	.	.	no
H110	C110	C111	H111	-0.68	.	.	.	no
C19	C110	C111	H111	179.41	.	.	.	no
N12	C113	C114	H114'	-170.04	.	.	.	no
N12	C113	C114	H114"	69.87	.	.	.	no
N12	C113	C114	H114	-50.02	.	.	.	no
C115	C113	C114	H114'	64.56	.	.	.	no
C115	C113	C114	H114"	-55.53	.	.	.	no
C115	C113	C114	H114	-175.42	.	.	.	no
H113	C113	C114	H114'	-52.60	.	.	.	no
H113	C113	C114	H114"	-172.70	.	.	.	no
H113	C113	C114	H114	67.41	.	.	.	no
N12	C113	C115	H115'	171.78	.	.	.	no
N12	C113	C115	H115"	51.82	.	.	.	no
N12	C113	C115	H115	-68.20	.	.	.	no
C114	C113	C115	H115'	-62.65	.	.	.	no
C114	C113	C115	H115"	177.39	.	.	.	no
C114	C113	C115	H115	57.36	.	.	.	no
H113	C113	C115	H115'	54.54	.	.	.	no
H113	C113	C115	H115"	-65.42	.	.	.	no
H113	C113	C115	H115	174.55	.	.	.	no
N12	C116	C117	H117'	170.10	.	.	.	no
N12	C116	C117	H117"	50.11	.	.	.	no
N12	C116	C117	H117	-69.93	.	.	.	no
C118	C116	C117	H117'	-63.93	.	.	.	no
C118	C116	C117	H117"	176.07	.	.	.	no
C118	C116	C117	H117	56.04	.	.	.	no
H116	C116	C117	H117'	52.56	.	.	.	no
H116	C116	C117	H117"	-67.43	.	.	.	no
H116	C116	C117	H117	172.54	.	.	.	no

N12	C116	C118	H118'	-177.84	.	.	.	no
N12	C116	C118	H118"	62.14	.	.	.	no
N12	C116	C118	H118	-57.86	.	.	.	no
C117	C116	C118	H118'	55.76	.	.	.	no
C117	C116	C118	H118"	-64.26	.	.	.	no
C117	C116	C118	H118	175.75	.	.	.	no
H116	C116	C118	H118'	-60.76	.	.	.	no
H116	C116	C118	H118"	179.22	.	.	.	no
H116	C116	C118	H118	59.23	.	.	.	no
O1	C119	C120	H120'	92.88	.	.	.	no
O1	C119	C120	H120	-146.28	.	.	.	no
H119'	C119	C120	C121	93.30	.	.	.	no
H119'	C119	C120	H120'	-147.13	.	.	.	no
H119'	C119	C120	H120	-26.28	.	.	.	no
H119	C119	C120	C121	-146.68	.	.	.	no
H119	C119	C120	H120'	-27.10	.	.	.	no
H119	C119	C120	H120	93.74	.	.	.	no
C119	C120	C121	H121'	-91.07	.	.	.	no
C119	C120	C121	H121	148.43	.	.	.	no
H120'	C120	C121	C122	-90.99	.	.	.	no
H120'	C120	C121	H121'	149.32	.	.	.	no
H120'	C120	C121	H121	28.82	.	.	.	no
H120	C120	C121	C122	148.20	.	.	.	no
H120	C120	C121	H121'	28.51	.	.	.	no
H120	C120	C121	H121	-91.99	.	.	.	no
C120	C121	C122	H122'	-140.02	.	.	.	no
C120	C121	C122	H122	100.24	.	.	.	no
H121'	C121	C122	O1	99.83	.	.	.	no
H121'	C121	C122	H122'	-20.34	.	.	.	no
H121'	C121	C122	H122	-140.09	.	.	.	no
H121	C121	C122	O1	-139.62	.	.	.	no
H121	C121	C122	H122'	100.21	.	.	.	no
H121	C121	C122	H122	-19.54	.	.	.	no
C26	C21	C22	C23	0.0(7)	.	.	.	no
B2	C21	C22	C23	174.7(5)	.	.	.	no
C22	C21	C26	C25	0.0(7)	.	.	.	no
B2	C21	C26	C25	-174.9(5)	.	.	.	no
C22	C21	B2	C27	142.1(5)	.	.	.	no
C22	C21	B2	C213	-98.5(5)	.	.	.	no
C22	C21	B2	C219	23.4(6)	.	.	.	no
C26	C21	B2	C27	-43.4(6)	.	.	.	no
C26	C21	B2	C213	76.0(5)	.	.	.	no
C26	C21	B2	C219	-162.1(4)	.	.	.	no
C21	C22	C23	C24	0.0(8)	.	.	.	no
C22	C23	C24	C25	0.2(8)	.	.	.	no
C23	C24	C25	C26	-0.2(8)	.	.	.	no
C24	C25	C26	C21	0.1(8)	.	.	.	no
C212	C27	C28	C29	-2.9(7)	.	.	.	no
B2	C27	C28	C29	-179.6(5)	.	.	.	no
C28	C27	B2	C21	-35.7(6)	.	.	.	no
C28	C27	B2	C213	-150.3(5)	.	.	.	no
C28	C27	B2	C219	87.3(5)	.	.	.	no
C212	C27	B2	C21	147.9(5)	.	.	.	no
C212	C27	B2	C213	33.3(6)	.	.	.	no
C212	C27	B2	C219	-89.1(5)	.	.	.	no
C28	C27	C212	C211	2.6(8)	.	.	.	no
B2	C27	C212	C211	179.3(5)	.	.	.	no
C27	C28	C29	C210	1.5(8)	.	.	.	no
C28	C29	C210	C211	0.6(9)	.	.	.	no
C29	C210	C211	C212	-1.0(8)	.	.	.	no
C210	C211	C212	C27	-0.7(8)	.	.	.	no

```
 C218    C213    B2      C219       -33.0(5)     .      .      .      .   no
 C214    C213    C218    C217        -0.8(6)     .      .      .      .   no
 C214    C213    B2      C27         33.3(6)     .      .      .      .   no
 C214    C213    B2      C219       151.9(4)     .      .      .      .   no
 C218    C213    B2      C27       -151.6(4)     .      .      .      .   no
 C218    C213    C214    C215         0.2(7)     .      .      .      .   no
 B2      C213    C214    C215       175.7(4)     .      .      .      .   no
 B2      C213    C218    C217      -176.3(4)     .      .      .      .   no
 C214    C213    B2      C21        -85.6(5)     .      .      .      .   no
 C218    C213    B2      C21         89.5(5)     .      .      .      .   no
 C213    C214    C215    C216         1.0(8)     .      .      .      .   no
 C214    C215    C216    C217        -1.5(8)     .      .      .      .   no
 C215    C216    C217    C218         0.9(7)     .      .      .      .   no
 C216    C217    C218    C213         0.3(7)     .      .      .      .   no
 C220    C219    C224    C223         2.8(6)     .      .      .      .   no
 B2      C219    C224    C223       179.0(4)     .      .      .      .   no
 B2      C219    C220    C221      -177.7(4)     .      .      .      .   no
 C224    C219    B2      C21         34.7(6)     .      .      .      .   no
 C224    C219    B2      C27        -86.6(5)     .      .      .      .   no
 C224    C219    B2      C213       151.7(4)     .      .      .      .   no
 C220    C219    B2      C21       -149.4(4)     .      .      .      .   no
 C220    C219    B2      C27         89.3(5)     .      .      .      .   no
 C220    C219    B2      C213       -32.5(6)     .      .      .      .   no
 C224    C219    C220    C221        -1.4(7)     .      .      .      .   no
 C219    C220    C221    C222        -1.7(8)     .      .      .      .   no
 C220    C221    C222    C223         3.5(8)     .      .      .      .   no
 C221    C222    C223    C224        -2.2(7)     .      .      .      .   no
 C222    C223    C224    C219        -1.1(7)     .      .      .      .   no

loop_
_geom_contact_atom_site_label_1
_geom_contact_atom_site_label_2
_geom_contact_distance
_geom_contact_site_symmetry_1
_geom_contact_site_symmetry_2
_geom_contact_publ_flag
 V1      H114"        3.2143                    .      .                  no
 V1      H115         3.2008                    .      .                  no
 O1      N11        2.762(5)                    .      .                  no
 O1      N12        2.956(6)                    .      .                  no
 O1      C13        3.358(8)                    .      .                  no
 O1      C14        2.873(8)                    .      .                  no
 O1      C15        3.294(9)                    .      .                  no
 O1      H14          2.8193                    .      .                  no
 N11     O1         2.762(5)                    .      .                  no
 N11     N12        2.745(5)                    .      .                  no
 N11     C11        2.839(9)                    .      .                  no
 N11     C15        2.940(7)                    .      .                  no
 N11     C113       3.110(6)                    .      .                  no
 N11     C114       3.184(7)                    .      .                  no
 N11     C115       3.156(7)                    .      .                  no
 N11     C122       3.110(7)                    .      .                  no
 N12     C13        3.279(7)                    .      .                  no
 N12     O1         2.956(6)                    .      .                  no
 N12     N11        2.745(5)                    .      .                  no
 N12     C12        3.078(7)                    .      .                  no
 N11     H11          2.9093                    .      .                  no
 N11     H115         2.4615                    .      .                  no
 N11     H122         2.9306                    .      .                  no
 N11     H114"        2.5078                    .      .                  no
 C11     N11        2.839(9)                    .      .                  no
```

C11	C13	2.217(10)	.	.	no
C11	C14	2.207(11)	.	.	no
C12	C14	2.181(11)	.	.	no
C12	C15	2.210(9)	.	.	no
C12	N12	3.078(7)	.	.	no
C12	C116	3.342(8)	.	.	no
C13	C116	3.328(8)	.	.	no
C13	C211	3.541(9)	.	1_655	no
C13	C11	2.217(10)	.	.	no
C13	C15	2.182(11)	.	.	no
C13	O1	3.358(8)	.	.	no
C13	N12	3.279(7)	.	.	no
C14	O1	2.873(8)	.	.	no
C14	C12	2.181(11)	.	.	no
C14	C119	3.438(11)	.	.	no
C14	C11	2.207(11)	.	.	no
C15	C13	2.182(11)	.	.	no
C15	C12	2.210(9)	.	.	no
C15	O1	3.294(9)	.	.	no
C15	N11	2.940(7)	.	.	no
C19	C110	3.597(7)	.	2_756	no
C22	C224	3.148(7)	.	.	no
C26	C28	3.236(7)	.	.	no
C26	C214	3.494(7)	.	.	no
C28	C26	3.236(7)	.	.	no
C110	C19	3.597(7)	.	2_756	no
C110	C117	3.500(8)	.	2_766	no
C11	H15	2.0672	.	.	no
C11	H12	2.1147	.	.	no
C12	H117"	3.0827	.	.	no
C12	H116	2.8735	.	.	no
C12	H14	3.0954	.	.	no
C12	H13	2.0359	.	.	no
C12	H11	2.1251	.	.	no
C13	H116	2.5722	.	.	no
C13	H15	3.0961	.	.	no
C13	H14	2.0488	.	.	no
C13	H12	2.0428	.	.	no
C14	H12	3.0976	.	.	no
C14	H13	2.0446	.	.	no
C114	N11	3.184(7)	.	.	no
C14	H119'	3.0384	.	.	no
C14	H15	2.0485	.	.	no
C115	N11	3.156(7)	.	.	no
C15	H13	3.0962	.	.	no
C15	H14	2.0515	.	.	no
C15	H23	3.0914	.	1_645	no
C115	C117	3.513(8)	.	.	no
C15	H11	2.0829	.	.	no
C15	H114'	2.8525	.	1_655	no
C16	H115	2.7865	.	.	no
C16	H112	2.9801	.	2_756	no
C16	H114"	2.9865	.	.	no
C17	H114"	3.0810	.	.	no
C17	H122	3.0297	.	.	no
C117	C115	3.513(8)	.	.	no
C17	H22	3.0440	.	1_545	no
C117	C110	3.500(8)	.	2_766	no
C19	H223	3.0588	.	2_666	no
C21	H224	2.8628	.	.	no
C21	H28	2.7784	.	.	no

C22	H224	2.7135	.	.	no
C22	H112"	3.0628	.	2_666	no
C22	H122	3.0564	.	1_565	no
C22	H17	2.8280	.	1_565	no
C122	C218	3.541(7)	.	1_545	no
C122	C217	3.502(9)	.	1_545	no
C23	H122	3.0914	.	1_565	no
C25	H121	3.0323	.	1_565	no
C25	H216	3.0205	.	1_455	no
C26	H28	2.9233	.	.	no
C26	H121	2.9102	.	1_565	no
C27	H214	2.7363	.	.	no
C27	H13	2.9960	.	1_455	no
C27	H26	2.7812	.	.	no
C28	H116	2.9918	.	1_455	no
C28	H120	3.0301	.	2_665	no
C28	H26	2.9104	.	.	no
C28	H13	2.9504	.	1_455	no
C29	H116	2.8504	.	1_455	no
C29	H13	2.8851	.	1_455	no
C110	H223	2.9731	.	2_666	no
C111	H223	3.0953	.	2_666	no
C211	C211	3.589(9)	.	2_665	no
C211	C13	3.541(9)	.	1_455	no
C111	H112	3.0253	.	2_756	no
C111	H115	3.0828	.	.	no
C112	H15	2.8291	.	2_756	no
C212	C214	3.120(7)	.	.	no
C113	H118"	2.6632	.	.	no
C113	H117	2.7367	.	.	no
C214	C26	3.494(7)	.	.	no
C214	C212	3.120(7)	.	.	no
C114	H23	2.9748	.	1_545	no
C115	H221	3.0857	.	.	no
C117	H115"	3.0117	.	.	no
C117	H113	2.6461	.	.	no
C117	H110	3.0141	.	2_766	no
C217	C122	3.502(9)	.	1_565	no
C118	H212	2.9451	.	.	no
C218	C122	3.541(7)	.	1_565	no
C118	H119	2.9299	.	.	no
C218	C220	3.144(7)	.	.	no
C118	H113	2.5829	.	.	no
C118	H29	3.0259	.	1_655	no
C119	H118	3.0311	.	.	no
C120	H26	2.9610	.	2_665	no
C220	C218	3.144(7)	.	.	no
C121	H25	3.0513	.	2_665	no
C122	H17	3.0067	.	.	no
C224	C22	3.148(7)	.	.	no
C210	H13	2.8183	.	1_455	no
C210	H119'	2.9897	.	1_455	no
C211	H211	2.9626	.	2_665	no
C211	H13	2.7836	.	1_455	no
C212	H13	2.8397	.	1_455	no
C212	H214	2.6786	.	.	no
C213	H212	2.7626	.	.	no
C213	H220	2.7501	.	.	no
C214	H212	2.7184	.	.	no
C215	H121'	3.0474	.	1_565	no
C216	H121'	2.9311	.	1_565	no

C217	H117'	3.0600	.	.	no
C217	H122'	2.7157	.	1_565	no
C218	H220	2.7043	.	.	no
C218	H122'	2.9728	.	1_565	no
C219	H22	2.7638	.	.	no
C219	H218	2.7968	.	.	no
C220	H218	2.7139	.	.	no
C220	H117	3.0828	.	.	no
C222	H12	2.9407	.	1_455	no
C222	H112'	3.0152	.	1_565	no
C223	H12	2.8621	.	1_455	no
C223	H117"	3.0138	.	1_455	no
C224	H22	2.6009	.	.	no
H112'	C222	3.0152	.	1_545	no
H112'	H18	2.3568	.	.	no
H112"	C22	3.0628	.	2_666	no
H114'	H115'	2.5764	.	.	no
H114'	C15	2.8525	.	1_455	no
H114"	V1	3.2143	.	.	no
H114"	N11	2.5078	.	.	no
H114"	C17	3.0810	.	.	no
H114"	H115	2.4633	.	.	no
H114"	C16	2.9865	.	.	no
H115'	H221	2.5890	.	.	no
H115'	H114'	2.5764	.	.	no
H115"	H115"	2.5714	.	2_766	no
H115"	C117	3.0117	.	.	no
H117'	C217	3.0600	.	.	no
H117'	H118'	2.5008	.	.	no
H117"	C223	3.0138	.	1_655	no
H117"	C12	3.0827	.	.	no
H117"	H12	2.3764	.	.	no
H118'	H29	2.5701	.	1_655	no
H118'	H117'	2.5008	.	.	no
H118"	C113	2.6632	.	.	no
H118"	H117	2.5047	.	.	no
H118"	H212	2.3973	.	.	no
H118"	H113	2.0273	.	.	no
H118"	H220	2.4025	.	.	no
H11	H111	2.4192	.	.	no
H11	H221	2.4807	.	2_766	no
H119'	C210	2.9897	.	1_655	no
H119'	H210	2.4723	.	1_655	no
H119'	H14	2.5254	.	.	no
H119'	C14	3.0384	.	.	no
H12	H117"	2.3764	.	.	no
H12	C223	2.8621	.	1_655	no
H12	C222	2.9407	.	1_655	no
H120'	H26	2.5031	.	2_665	no
H13	C29	2.8851	.	1_655	no
H13	C210	2.8183	.	1_655	no
H13	C211	2.7836	.	1_655	no
H13	C212	2.8397	.	1_655	no
H13	H116	2.2121	.	.	no
H13	C27	2.9960	.	1_655	no
H13	C28	2.9504	.	1_655	no
H121'	C216	2.9311	.	1_545	no
H121'	C215	3.0474	.	1_545	no
H14	H119'	2.5254	.	.	no
H14	H24	2.4752	.	1_645	no
H122'	C217	2.7157	.	1_545	no

H122'	C218	2.9728	.	1_545	no
H15	H23	2.5144	.	1_645	no
H15	C112	2.8291	.	2_756	no
H15	H112	2.4825	.	2_756	no
H17	C122	3.0067	.	.	no
H17	H22	2.3455	.	1_545	no
H17	C22	2.8280	.	1_545	no
H17	H122	2.2495	.	.	no
H18	H112'	2.3568	.	.	no
H22	H224	2.3189	.	.	no
H22	C17	3.0440	.	1_565	no
H22	C219	2.7638	.	.	no
H22	C224	2.6009	.	.	no
H22	H17	2.3455	.	1_565	no
H23	H15	2.5144	.	1_465	no
H23	C15	3.0914	.	1_465	no
H23	C114	2.9748	.	1_565	no
H24	H14	2.4752	.	1_465	no
H25	H121	2.4157	.	2_665	no
H25	C121	3.0513	.	2_665	no
H26	C27	2.7812	.	.	no
H26	C28	2.9104	.	.	no
H26	C120	2.9610	.	2_665	no
H26	H120'	2.5031	.	2_665	no
H28	C21	2.7784	.	.	no
H28	C26	2.9233	.	.	no
H29	H118'	2.5701	.	1_455	no
H29	H210	2.3508	.	2_565	no
H29	C118	3.0259	.	1_455	no
H110	H112	2.5816	.	.	no
H110	C117	3.0141	.	2_766	no
H111	H11	2.4192	.	.	no
H112	H110	2.5816	.	.	no
H112	C16	2.9801	.	2_756	no
H112	C111	3.0253	.	2_756	no
H112	H15	2.4825	.	2_756	no
H113	C117	2.6461	.	.	no
H113	C118	2.5829	.	.	no
H113	H118"	2.0273	.	.	no
H113	H117	2.1444	.	.	no
H113	H220	2.5980	.	.	no
H113	H221	2.5801	.	.	no
H115	H114"	2.4633	.	.	no
H115	V1	3.2008	.	.	no
H115	N11	2.4615	.	.	no
H115	C16	2.7865	.	.	no
H115	C111	3.0828	.	.	no
H116	C28	2.9918	.	1_655	no
H116	C12	2.8735	.	.	no
H116	C13	2.5722	.	.	no
H116	C29	2.8504	.	1_655	no
H116	H13	2.2121	.	.	no
H117	H113	2.1444	.	.	no
H117	C113	2.7367	.	.	no
H117	C220	3.0828	.	.	no
H117	H118"	2.5047	.	.	no
H117	H220	2.3403	.	.	no
H118	C119	3.0311	.	.	no
H118	H119	2.0772	.	.	no
H119	C118	2.9299	.	.	no
H119	H118	2.0772	.	.	no

```
 H120    C28          3.0301                    .     2_665                no
 H120    H216         2.5699                    .     2_765                no
 H121    C25          3.0323                    .     1_545                no
 H121    C26          2.9102                    .     1_545                no
 H121    H25          2.4157                    .     2_665                no
 H122    N11          2.9306                    .       .                  no
 H122    C17          3.0297                    .       .                  no
 H122    C22          3.0564                    .     1_545                no
 H122    C23          3.0914                    .     1_545                no
 H122    H17          2.2495                    .       .                  no
 H210    H119'        2.4723                    .     1_455                no
 H210    H29          2.3508                    .     2_565                no
 H211    C211         2.9626                    .     2_665                no
 H211    H211         2.5461                    .     2_665                no
 H212    C118         2.9451                    .       .                  no
 H212    C213         2.7626                    .       .                  no
 H212    C214         2.7184                    .       .                  no
 H212    H118"        2.3973                    .       .                  no
 H212    H214         2.4912                    .       .                  no
 H214    C27          2.7363                    .       .                  no
 H214    C212         2.6786                    .       .                  no
 H214    H212         2.4912                    .       .                  no
 H216    C25          3.0205                    .     1_655                no
 H216    H120         2.5699                    .     2_765                no
 H218    C219         2.7968                    .       .                  no
 H218    C220         2.7139                    .       .                  no
 H218    H220         2.4732                    .       .                  no
 H220    C213         2.7501                    .       .                  no
 H220    C218         2.7043                    .       .                  no
 H220    H118"        2.4025                    .       .                  no
 H220    H113         2.5980                    .       .                  no
 H220    H117         2.3403                    .       .                  no
 H220    H218         2.4732                    .       .                  no
 H221    C115         3.0857                    .       .                  no
 H221    H115'        2.5890                    .       .                  no
 H221    H113         2.5801                    .       .                  no
 H221    H11          2.4807                    .     2_766                no
 H223    C19          3.0588                    .     2_666                no
 H223    C110         2.9731                    .     2_666                no
 H223    C111         3.0953                    .     2_666                no
 H224    C21          2.8628                    .       .                  no
 H224    C22          2.7135                    .       .                  no
 H224    H22          2.3189                    .       .                  no

loop_
_geom_hbond_atom_site_label_D
_geom_hbond_atom_site_label_H
_geom_hbond_atom_site_label_A
_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_site_symmetry_A
_geom_hbond_publ_flag
#
#D   H   A   D - H  H...A   D...A    D - H...A  symm(A)
#
C114    H114"   N11         0.9800     2.5100   3.184(7)     126.00     .   yes
C115    H115    N11         0.9800     2.4600   3.156(7)     128.00     .   yes

#===END of Crystallographic Information File
```